Modeling Phase Transformations with Strength in Zirconium

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The previously developed free energy approach to modeling materials with phase transformations has been updated to include a linear hardening plasticity algorithm and improved kinetics more representative of the observed behavior of zirconium. The material model has been implemented into a 3D Lagrangian finite-element code.

The plasticity is based on the assumption that in a multiphase material, the phase that has the lowest yield strength will receive all of the deformation. An implicit formulation for the deviatoric stress invariant when the yield condition is satisfied is given by

$$\tau = \frac{\sigma_y^{\min} + \sigma_y^{\min} / 3\bar{\mu}\xi^{\min}\tau^*}{1+\sigma_y^{\min} / 3\bar{\mu}\xi^{\min}}, \qquad (1)$$

where the minimum yield surface value is

$$\sigma_y^{\min} = \min(\sigma_y^{\alpha}, \sigma_y^{\beta}, \sigma_y^{\gamma}),$$

the mass fraction of the minimum nonzero phase is $\xi^{\min} = \min(\xi^{\alpha}, \xi^{\beta}, \xi^{\omega})$,

the composite shear modulus is

$$\bar{\mu} = \sum_{k=\alpha,\beta,\omega} \frac{1}{\xi_k / \mu_k},$$

and τ* is the trial stress. The trial stress is the stress invariant that would be realized if all the deformation was accommodated elastically,

$$\tau^* = \sqrt{\tfrac{3}{2}\underline{\underline{s}}^* : \underline{\underline{s}}^*}, \quad \underline{\underline{s}}^* = 2\bar{\mu}\underline{\underline{D}}', \qquad (2)$$

where $\underline{\underline{s}}^*$ is the trial deviatoric Cauchy stress tensor, and $\underline{\underline{D}}'$ is the deviatoric rate of deformation tensor. The deviatoric stress is

$$\underline{\underline{s}} = \underline{\underline{s}}^* \frac{\tau}{\tau^*}. \qquad (3)$$

The yield surfaces for each phase evolve using a linear hardening rule in equivalent plastic strain.

The transformation rate (for the α–ω phase transition) is given by phenomenological model

$$\dot{\xi} = (1-\xi_\omega)\nu \frac{G_\alpha - G_\omega}{B} \exp\left(\frac{G_\alpha - G_\omega}{B}\right)^2 \qquad (4)$$

where G_{phase} is the Gibbs free energy for each phase and (ν, B) are material constants.

The material model was coded in FORTRAN 90 in a modular form for simplified implementation into Advanced Simulation and Computing codes. The modular form was inserted into a 3D Lagrangian finite-element test-bed code for verification.

A plate on plate impact problem was used to verify the implementation. Both 1D and 3D calculations were performed for a sapphire plate impacting an alpha phase zirconium plate at 658 m/s. Figure 1 shows the evolution of the mass fractions of each phase, the yield stresses of each phase, and the von Mises stress as a function of time for the one dimensional plate on plate impact. For the 3D simulation, Fig. 2 compares the velocity and phase distribution for three times.

[1] C.W. Greeff, P.A. Rigg, M.D. Knudson, R.S. Hixson, and G.T. Gray III, "Modeling Dynamic Phase Transitions in Ti and Zr," AIP, **CP706**, 209-212 (2003)
[2] F.L. Addessio, Q.H. Zuo, and T.A. Mason, and L.C. Brinson, "A Model for High-Strain-Rate Deformation of Uranium-Niobium Alloys," *J. Appl. Phys.*, **93**, 12, 9644 (2003).

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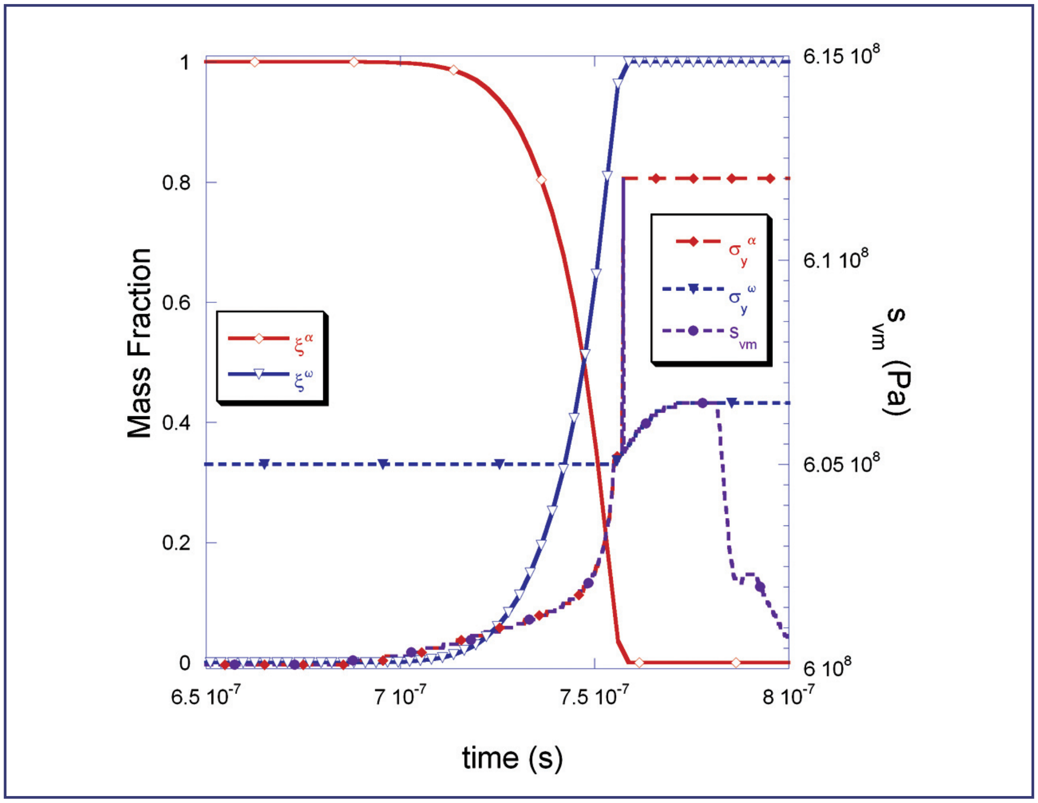

Figure 1—
One-dimensional plate on plate impact: mass fraction of each phase and deviatoric stress evolution in time.

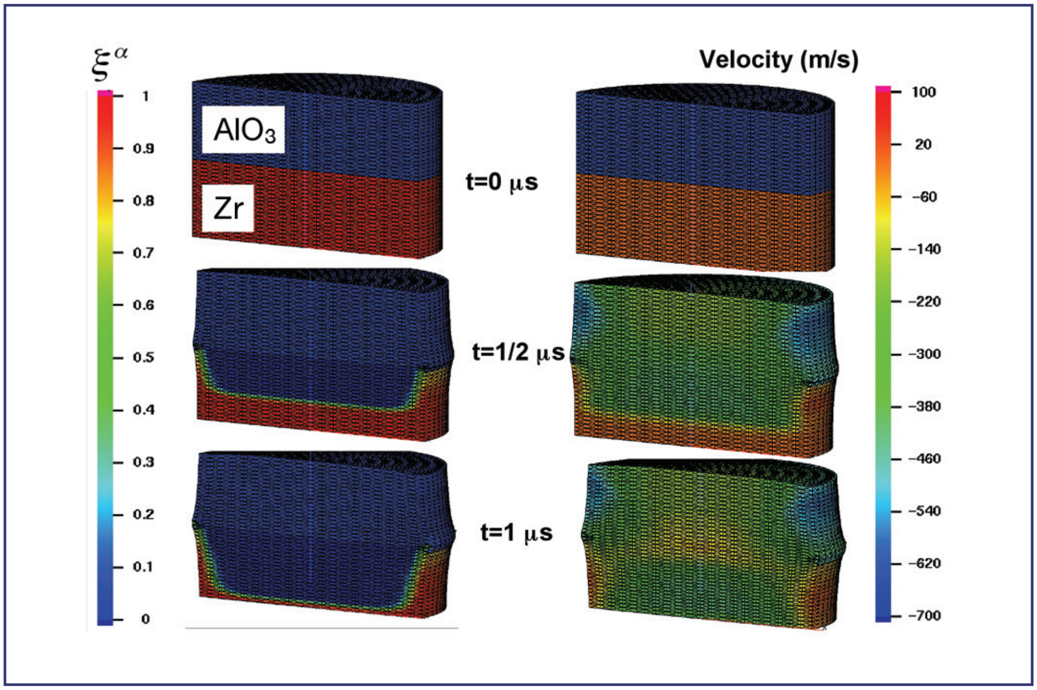

Figure 2—
Three-dimensional plate on plate impact: velocity and phase transition waves.

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